

RECOVERY, A Mathematical Model to Predict the Temporal Response of Surface Water to Contaminated Sediments

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Final report

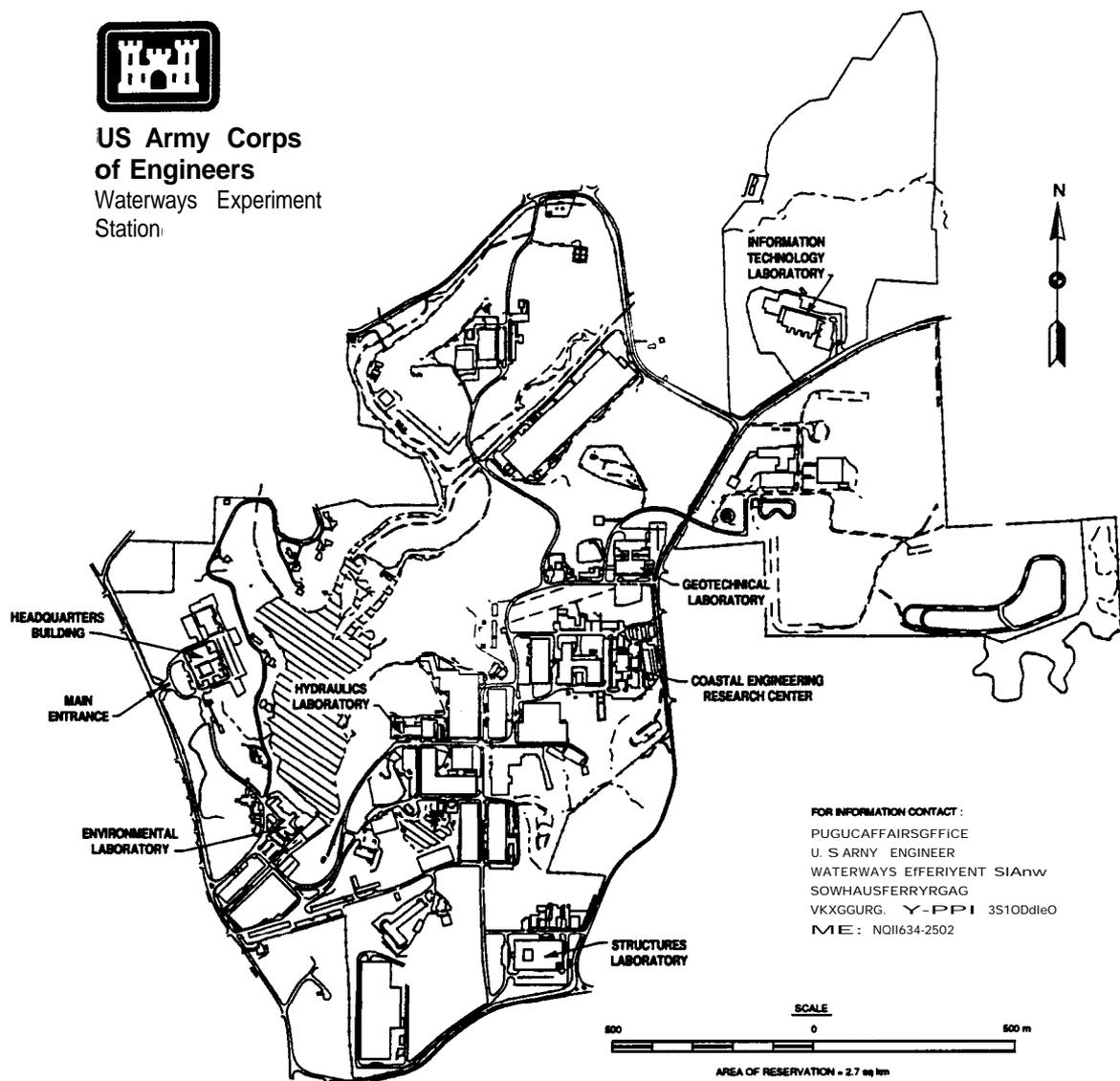
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Prepared for U.S. Army Corps of Engineers
Washington, DC 20314-1 000
U.S. Army Engineer Division, New England
Waltham, MA 02254-9149
and U.S. Army Engineer District, New York
New York, NY 10278-0090



**US Army Corps
of Engineers**

Waterways Experiment
Station



Waterways Experiment Station Cataloging-in-Publication Data

RECOVERY : a mathematical model to predict the temporal response of surface water to contaminated sediments /by Jean M. Boyer . . . [et al.] ; prepared for U.S. Army Corps of Engineers, U.S. Army Engineer Division, New England and U.S. Army Engineer District, New York.

61 p. : ill. ; 28 cm. — (Technical report ; W-94-4)

Includes bibliographic references.

1. Water quality — Measurement — Data processing. 2. RECOVERY (Computer program) 3. Marine sediments — Environmental aspects. 4. Sediments (Geology) — Environmental aspects. I. Boyer, Jean M. II. United States. Army. Corps of Engineers. III. United States. Army. Corps of Engineers. New England Division. IV. United States. Army. Corps of Engineers. New York District. V. U.S. Army Engineer Waterways Experiment Station. VI. Water Quality Research Program. VII. Title: A mathematical model to predict the temporal response of surface water to contaminated sediments. VIII. Series: Technical report (U.S. Army Engineer Waterways Experiment Station) ; W-94-4.

TA7 W34 no.W-94-4

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Preface

The work reported herein was sponsored by the U.S. Army Engineer Division, New England, U.S. Army Engineer District, New York, and by the Headquarters, U.S. Army Corps of Engineers (HQUSACE), as part of the Water Quality Research Program (WQRP), Work Unit 32808. The WQRP is assigned to the U.S. Army Engineer Waterways Experiment Station (WES) under the purview of the Environmental Laboratory (EL). Funding was provided under Department of the Army Appropriation No. 96X3121, General Investigation. The WQRP is managed under the Environmental Resources Research and Assistance Programs (ERRAP), Mr. J. L. Decell, Manager. Mr. Robert C. Gunkel was Assistant Manager, ERRAP, for the WQRP. Technical Monitors during this study were Mr. Frederick B. Juhle, Mr. Rixie Hardy, and Dr. John Bushman, HQUSACE.

This report provides documentation of the RECOVERY model (Version 1 .O), including mathematical formulations, computational algorithms, a user's guide, and a confirmation application. The Principal Investigator for this study was Dr. Carlos E. Ruiz, Water Quality and Contaminant Modeling Branch (WQCMB), Environmental Processes and Effects Division (EPED) EL. Model development was conducted under contract to the Center for Advanced Decision Support for Water and Environmental Systems (CADSWES), University of Colorado, Boulder, CO. Dr. Steven C. Chapra and Ms. Jean M. Boyer of CADSWES performed the original model development. Drs. Ruiz and Mark S. Dortch of WQCMB provided guidance during development.

This report was prepared by Ms. Boyer and Drs. Chapra, Ruiz, and Dortch. This study was conducted under the direct supervision of Dr. Dortch, Chief, WQCMB, and under the general supervision of Mr. Donald L. Robey, Chief, EPED, and Dr. John W. Keeley, Director, EL. This report was reviewed by Drs. Douglas Gunnison, Environmental Processes and Effects Branch, EPED, and Carl F. Cerco, WQCMB.

At the time of publication of this report, Director of WES was Dr. Robert W. Whalin. Commander was COL Bruce K. Howard, EN.

This report should be cited as follows:

Boyer, J. M., Chapra, S. C., Ruiz, C. E., and Dortch, M. S. (1994). "RECOVERY, a mathematical model to predict the temporal response of surface water to contaminated sediments," Technical Report W-94-4, U.S. Army Engineer Waterways Experiment Station, Vicksburg, MS.

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1 Introduction

Toxic substances are known to associate strongly with fine-grain particulate matter. Consequently, it is not surprising that toxicants tend to accumulate in the bottom sediments of natural waters. An important question in environmental impact assessment is to what extent do these contaminated sediments influence overlying waters.

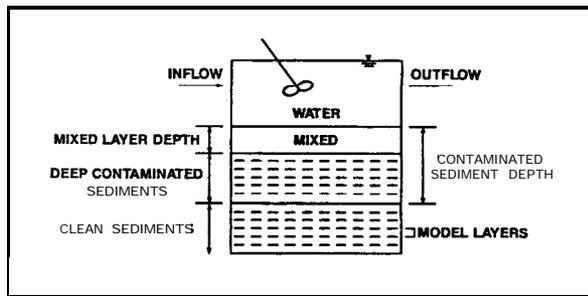
The report herein describes a modeling framework that is designed to assess the impact of contaminated bottom sediments on surface waters. The analysis is limited to cases where the overlying water is well mixed. In addition, the contaminant is assumed to be organic and to follow linear equilibrium sorption and first-order decay kinetics.

The framework is implemented via a personal computer software package-RECOVERY. It is designed for interactive implementation and is self-documented. RECOVERY allows the user to rapidly generate and analyze recovery scenarios for contaminated systems. The software includes graphical displays and can be run on IBM-PC compatible microcomputers.

This report provides supplemental documentation, including a mathematical description of the model, its computational algorithm, and a confirmation implementation. It also includes a user's guide.

2 Model Description

The present model is an application and extension of frameworks developed previously (Chapra 1982, 1986; Chapra and Reckhow 1983). As in Figures 1 and 2, the system is idealized as a well-mixed surface water layer underlain by a vertically stratified sediment column. The sediment is well mixed horizontally, but segmented vertically into a well-mixed surface layer and a deep sediment. The latter, in turn, is segmented into contaminated and uncontaminated regions. The specification of a mixed surface layer is included because an unconsolidated layer is often observed at the surface of sediments because of a number of processes, including bioturbation and mechanical mixing.



A list of assumptions used in the development of this model can be found in Table 1. Also, nomenclature used in this report is listed in Appendix A.

Figure 1. Physical configuration of RECOVERY

Contaminant Mass Balances

A mass balance for the contaminant in the water can be written as

$$V_w \frac{dc_w}{dt} = Qc_i - Qc_w - k_w V_w c_w - k_v V_w c_w - v_s A_w F_{pw} c_w + v_r A_m c_m + v_d A_m (F_{dp} c_m - F_{dw} c_w) \quad (1)$$

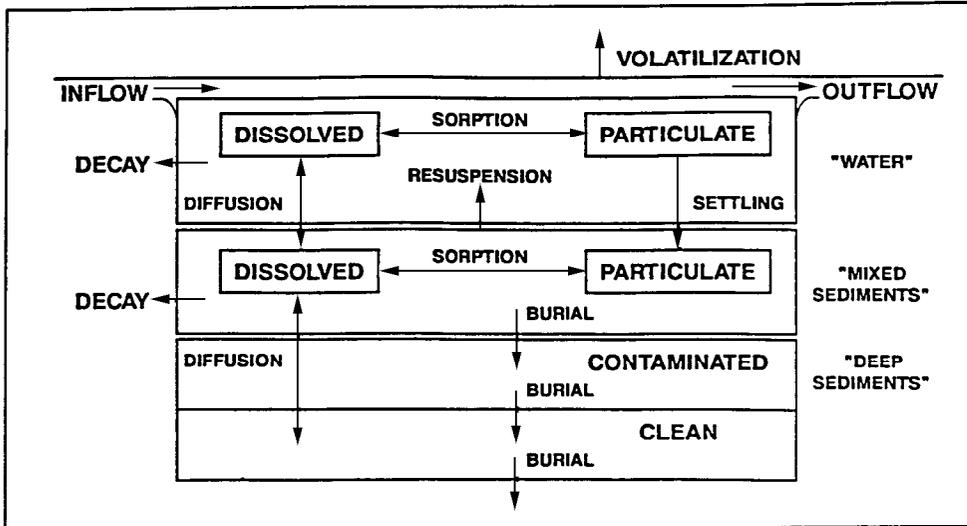


Figure 2. Schematic of RECOVERY

Table 1 List of Assumptions Used in Development of RECOVERY
Contaminant is of organic nature.
Water body is well mixed.
Mixed layer is well mixed.
In the deep sediments, contaminant concentration varies in vertical direction only.
Initial concentration of compound in contaminated region is uniform throughout region.
Initial concentration of contaminant in region below contaminated region is zero.
Sediments are only source of contaminant to water body.
Contaminant follows a linear equilibrium sorption mechanism.
Contaminant decays according to first order kinetics.
There is no compaction in sediments.
System is isothermal.
Water body is at 25 °C.
Only single component mass transfer is described. Movement of contaminant is independent of presence of other contaminants.
Flow through is constant.

where

V_w = volume of water body, m^3

c_w and c_m = concentrations of toxicant in water and mixed sediments, respectively, $\mu g/m^3$

t = time, years

Q = flushing flow rate, $m^3/year$

c_i = inflow concentration, $\mu g/m^3$, which reflects both direct and tributary loadings (in the present version of the model, this concentration is assumed to be zero)

k_w = decay rate constant of contaminant in water, /year

k_v = volatilization rate of contaminant, /year

v_s = settling velocity of particulate matter, m/year

A_w and A_m = surface areas of water and mixed sediment, respectively, m^2

F_{pw} = fraction of contaminant in particulate form in water

v_r = resuspension velocity of sediments, m/year

v_d = diffusion mass transfer coefficient at sediment-water interface, m/year

F_{dp} = ratio of contaminant concentration in sediment pore water to contaminant concentration in total sediment

F_{dw} = fraction of contaminant in dissolved form in water

The initial condition for Equation 1 at $t = 0$ is $c_w = c_{w0}$.

A mass balance for the mixed-sediment layer can be written as

$$\begin{aligned}
 V_m \frac{dc_m}{dt} = & -k_m V_m c_m + v_s A_w F_{pw} c_w - v_r A_m c_m - v_b A_m c_m \\
 & + v_d A_m (F_{dw} c_w - F_{dp} c_m) + v_d A_m (F_{dp} c_s(0) - F_{dp} c_m)
 \end{aligned} \tag{2}$$

where

V_m = volume of mixed layer, m^3

k_m = decay rate constant of contaminant in mixed layer, /year

v_b = burial velocity, m/year

$c_s(0)$ = contaminant concentration at top of deep contaminated layer, $\mu g/m^3$

The initial condition for this equation at $t = 0$ is $c_m = c_{m0}$.

Both the deep contaminated and clean sediments can be modeled with one-dimensional advection-diffusion-decay equations of the form

$$\frac{\partial c_s}{\partial t} = \phi F_{dp} D_s \frac{\partial^2 c_s}{\partial z^2} - v_b \frac{\partial c_s}{\partial z} - k_s c_s \quad (3)$$

where

c_s = contaminant concentration in deep sediments, $\mu g/m^3$

ϕ = the sediment porosity

D_s = diffusion rate in sediment pore water, $m^2/year$

z = depth into sediment, m, where $z = 0$ at top of deep sediments

k_s = decay rate constant of contaminant in deep sediments, /year

The initial and boundary conditions for Equation 3 are as follows:

IC: at $t = 0$, $c_s = c_{s0}$ ($z_m < z < L$)

IC: at $t = 0$, $c_s = 0$ ($L < z < \infty$)

BC 1: at $z = z_m$, $J = J_{ms}$

BC 2: at $z = \infty$, $\frac{\partial c_s}{\partial z} = 0$

where

L = distance from top of mixed layer to bottom of contaminated layer

J = mass flux of contaminant, $\text{g}/(\text{m}^2\text{-year})$

J_{ms} = mass flux of contaminant from mixed layer to sediment layer,
 $\text{g}/(\text{m}^2\text{-year})$

The F 's in Equations 1-3 are dimensionless ratios that reflect how the contaminant partitions between solid matter and water assuming a linear sorption mechanism. Denoting the contaminant as A , they are defined as

$$F_{pw} = \frac{K_{dw}S_w}{1 + K_{dw}S_w}$$

$$= \left(\frac{\frac{\text{Mass of A (Particulate Form)}}{\text{Total Volume}}}{\frac{\text{Mass of A (Dissolved Form)} + \text{Mass of A (Particulate Form)}}{\text{Total Volume}}} \right)_{\text{Water Body}} \quad (4)$$

$$F_{dw} = 1 - F_{pw} = \frac{1}{1 + K_{dw}S_w}$$

$$= \left(\frac{\frac{\text{Mass of A (Dissolved Form)}}{\text{Total Volume}}}{\frac{\text{Mass of A (Dissolved Form)} + \text{Mass of A (Particulate Form)}}{\text{Total Volume}}} \right)_{\text{Water Body}} \quad (5)$$

$$F_{dp} = \frac{1}{\phi + K_{ds}(1 - \phi)\rho}$$

$$= \left(\frac{\frac{\text{Mass of A (Dissolved Form)}}{\text{Volume of Pore Water}}}{\frac{\text{Mass of A (Dissolved Form)} + \text{Mass of A (Particulate Form)}}{\text{Total Volume}}} \right)_{\text{Sediment}} \quad (6)$$

where

K_{dw} and K_{ds} = contaminant partition coefficient in water and sediments,
respectively, m^3/g

ρ = density of sediment solids, g/m^3

S_w = suspended solids concentration in water, g/m^3

Note that the model allows different values of this parameter to be employed in the mixed layer and the vertically segmented sediments (F_{dpm} and F_{dps}).

The decay rate constants k_w , k_m , and k_s represent all mechanisms for decay except volatilization, which is accounted for separately. These mechanisms include photolysis, hydrolysis, and bacterial degradation.

The mass transfer coefficient for diffusive sediment-water exchange is related to more fundamental parameters by

$$v_d = \frac{\phi D_s}{z'} \quad (7)$$

where

ϕ = porosity

D_s = diffusion coefficient in sediment pore water, m^2/year

z' = characteristic length over which gradient exists at sediment-water interface, m.

Note that a value of 1 cm is assumed for z' after Thomann and Mueller (1987). Also, D_s is related to molecular diffusivity D_m by the relation (Berner 1980; Manheim and Waterman 1974)

$$D_s = D_m \phi^2$$

Solids Budget

The velocity terms— v_s , v_r , and v_b —in Equations 1 and 2 are computed according to a steady-state mass balance for mixed-sediment layer solids as described by Chapra and Reckhow (1983). The mass balance is

$$0 = v_s A_w s_w - (v_r + v_b) A_m (1 - \phi) \rho_p \quad (8)$$

The framework assumes that suspended solids concentration s_w is given. Therefore, if two of the three velocities are specified, Equation 8 can be employed to calculate the third.

In addition to these transfer velocities, the other facet of the model related to the solids budget is the sediment porosity. Different porosities are allowed for the mixed layer and the deep sediments. Within these regions, porosity is constant. This means that compaction is not included.

Default Parameters

Several parameters in the above framework are provided by the software as default values. These are suggested values that represent first estimates. They can be easily modified by the user.

Volatilization rate

The volatilization rate is computed by

$$k_v = F_{dw} \frac{v_v}{z_w} \quad (9)$$

where v_v = a volatilization transfer coefficient, m/year, which can be computed according to the Whitman two-film theory as

$$v_v = \frac{K_l K_g H_e}{K_g H_e + K_l} \quad (10)$$

where H_e = a dimensionless Henry's coefficient that is related to the common form H_e' (atm m³/gmole) by

$$H_e = \frac{H_e'}{RT} \quad (11)$$

where

R = universal gas constant = 8.206×10^{-5} atm m³/(gmole-kelvins)

T = absolute temperature, kelvins.

A temperature of 298K (25 °C) is assumed in the model.

The parameter K_g is a gas-film mass transfer coefficient (m/year) that can be related to wind speed, U_w (m/s), and molecular weight, MW (g/gmole), by (Mills et al. 1982)

$$K_g = 61320 \left(\frac{18}{MW} \right)^{0.25} U_w \quad (12)$$

The parameter K_l is a liquid-film mass transfer coefficient (m/year) that can be related to wind speed, U_w (m/s), and molecular weight, MW (g/gmole), by (Mills et al. 1982; Banks 1975; Banks and Herrera 1977)

$$K_d = 365 \left(\frac{32}{MW} \right)^{0.25} (0.728U_w^{0.5} - 0.317U_w + 0.0372U_w^2) \quad (13)$$

Partition coefficient

The partition coefficient for organic contaminants is computed via (Karichhoff et al. 1979)

$$K_d = 0.617f_{oc}K_{ow} \quad (14)$$

where

f_{oc} = weight fraction of organic carbon in solid matter, **g-orgC/g**

K_{ow} = octanol-water partition coefficient, **(mg/m³-octanol)/(mg/m³-water)**

Note that the model assumes a default of 0.05 for f_{oc} .

Numerical Methods

The coupled set of differential equations is solved numerically. The two first-order ODEs, Equations 1 and 2, are solved using an adaptive-step-size, fourth-order Runge-Kutta method (Press et al. 1988). The partial differential equation is solved using the Crank-Nicolson technique (Chapra and Canale 1988).

The total number of years for which the model is run is determined by approximating the time required for the contaminant concentration in the water to decrease to 10 percent of the maximum value achieved. This is determined by using an analytical solution for the case where only the water and a single well-mixed layer are considered. This procedure has been found to be effective in approximating the total time.

3 Model Confirmation

The time variable model RECOVERY has been applied to analyze a field-scale experiment in which a flooded limestone quarry was dosed with equal quantities of the insecticides DDE (dichloro-diphenyldichloro-ethylene) and lindane (hexachlotocyclohexane). The same experiment was previously analyzed with a time variable model by Di Toro and Paquin (1983) with good results.

Study Area

The study was conducted in two flooded limestone quarries located near the town of Oolitic in Bedford County, Indiana. The quarries were allowed to flood naturally for 5 years before being dosed with the insecticides lindane and DDE. One quarry was experimentally dosed (quarry T), and the second was used as the control (quarry C) (Waybrant 1973).

Quarry T was 300 ft long, 135 ft wide, and an average of 50 ft. deep. Quarry T was the smaller of the two in area, with extremely clear water and generally flat bottom. The average Secchi disc reading for quarries C and T was 20 ft. Both quarries exhibited thermal stratification from March to November.

The relatively soft and slightly alkaline water found in the quarries tend to indicate mat the quarries received very little groundwater (Waybrant 1973). The water chemistry and physical characteristics of the quarries indicated that the quarries were primarily tilled with rainwater and runoff water that did not percolate through the limestone to the groundwater.

The bottom material in quarry T was made up of 3 to 5 cm of fine brownish gyttja underlaid by a white inorganic mixture of limestone dust and silica sand (Waybrant 1973). In general, the top sediment layers were aerobic. The mud layer contained on the average 1 percent sand, 42 percent silt, and 57 percent clay.

Overview

Quarry T was treated with the insecticides lindane and DDE at a concentration of 200 parts per trillion (ppt) to the epilimnion or 50 ppt overall (2.7764 g of DDE and 2.7752 g of lindane) (Waybrant 1973). The quarries were analyzed after the treatment, and the results showed that essentially all of the insecticides were initially released in the epilimnion. The quarries were periodically sampled, and the results are presented in Table 2. Both water and bottom sediments were analyzed for the insecticides DDE and lindane. The results for insecticides in the bottom sediment material are shown in Table 3.

Table 2 Concentrations of DDE and Lindane in Water Column		
Sampling Day	DDE, ppt, X ± SD	Lindane, ppt, X ± SD
1	44.0420 ± 16.336	47.270 ± 3.676
5	14.994 ± 3.429	62.792 ± 10.419
10	4.270 ± 2.066	60.828 ± 2.733
21	3.520 ± 1.768	58.874 ± 15.683
42	3.311 ± 1.324	50.418 ± 2.087
60	2.132 ± 0.613	29.852 ± 16.510
81	2.006 ± 0.163	32.939 ± 4.048
102	1.466 ± 0.163	34.577 ± 4.059
123	0.988 ± 0.220	25.440 ± 7.369
144	0.789 ± 0.171	23.189 ± 2.378
173	0.958 ± 0.163	21.318 ± 0.667
242	0.952 ± 0.103	20.284 ± 1.458

Note: SD = standard deviation; X = mean; ppt = parts per trillion (Waybrant 1973).

The concentration of DDE and lindane remaining in the water column after 5 days differed significantly (Table 2) showing different transport mechanisms by the two insecticides. After Day 1, a significant runoff event occurred in quarry T, washing a significant amount of sediment into the quarry. The suspended sediment load caused the DDE concentration in the water column to decrease as suspended solids, and the adsorbed DDE settled to the lake bottom. DDE hydrophobic properties cause affinity to suspended solids and organic matter, while lindane, a more polar compound, tends to have higher affinity for water.

Over the sampling period, an extremely rapid distribution of DDE in the water column was noted as opposed to an 87-percent retention of lindane in the surface layers (Waybrant 1973). The quarry underwent turnover at

Table 3 DDE and Lindane Concentration in Bottom Sediments					
Day	Depth, cm	DDE, ppb X ± SD	% of Total	Lindane, ppb X ± SD	% of Total
1	1.5 3.5 5.5	0.10		7.05 7.05	
5	1.5 3.5 5.5	18.66 ± 14.50	30.27	1.54 ± 0.14	2.50
10	1.5 3.5 5.5	22.28 ± 6.04 1.15 ± 1.49 <0.10	36.15 1.87	1.48 <0.05 <0.05	2.40
21	1.5 3.5 5.5	12.73 ± 11.30 0.28 ± 0.11	20.65 0.45	1.64 ± 0.43 1.04 ± 0.87	2.65
42	1.5 3.5 5.5	20.84 ± 5.53 0.14 <0.10	33.82 0.23	0.98 ± 1.36 <0.05	1.59
81	1.5 3.5 5.5	35.30 ± 27.45 <0.10 <0.10	57.27	1.13 ± 1.52 0.99 0.95 ± 0.57	1.83
123	1.5 3.5 5.5	27.27 ± 15.85 0.11 0.88 ± 1.06	45.24 0.18 1.43	1.87+1.77 2.46 ± 2.31 1.40 ± 0.97	3.03 3.99 2.63
173	1.5 3.5 5.5	30.92 ± 13.39 5.08 0.18	50.17 8.24	1.78 ± 1.60 2.15 ± <0.05	2.88 3.49
242	1.5 3.5 5.5	19.69 ± 2.80 0.31 ± 0.02 0.39 ± 0.45	31.95 0.50	<0.05 <0.05	
Note: SD = standard deviation; X = mean; ppb = park per billion (Waybrant 1973).					

Day 144, when the DDE and lindane distribution in the water column was essentially homogeneous. The lindane concentration in the water column decreases until Day 123, after which the insecticide concentration remains constant until the sample after the following spring.

DDE and lindane were both detected in the bottom sediments at significantly higher concentrations after the initial pesticide loading. However, the ultimate fate of both pesticides was considerably different. DDE, a more hydrophobic compound, was rapidly deposited in the bottom sediments (Table 3) while lindane concentration never reached the relatively high levels observed with DDE.

DDE peaked at 35 parts per billion (ppb) in the bottom sediments, while lindane levels did not exceed 2.5 ppb in the sediments. Both compounds

reached the highest level in the sediments between Days 81 and 123, lindane penetrating the lower depth of the bottom sediments while DDE remained mostly on the top layer.

Some important notes from the flooded quarry experiment were the significantly higher water column concentration of lindane, an order of magnitude above DDE at the end of the study. The reverse was true for the sediment concentration, with lindane penetrating to the deeper sediment layer of 3.5 to 5.5 cm. In addition, lindane profile in the sediment did not exhibit a pronounced vertical gradient.

Approximately 5 years after the initial dosing of the quarry on June 21, 1977, several sediment samples were collected and analyzed for DDE (Di Toro and Paquin 1983). The DDE concentration measured in that sampling event ranged from 3.4 to 11.2 ppb for one sample and from 2.9 to 4.2 ppb for another. The water column was sampled at the same time, but the detection limit of the analysis was 30 ppt (Di Toro and Paquin 1983). Sampling was not done for lindane in the 1977 sampling.

Rate Coefficients

To simulate the flooded quarry with the RECOVERY model, the basic assumptions of the model need to be satisfied. The first one, the water body is well mixed, might be satisfied after Day 23 (Table 2) and for sure at Day 144. For the application of RECOVERY, the simulation will begin between Days 81 and 123, a time where the pesticide profile looks fairly uniform. The second one, the sediments are the only source of the contaminant to the water body, is satisfied by Day 81 for DDE and Day 123 for lindane. At those days, the concentration in the sediment peaks for each of the simulated compounds. Once the concentration peaks in the sediment, the water cannot be a source of contaminant anymore (quasi-equilibrium is temporarily established) unless a considerable loss of contaminant is occurring in the sediments.

The third assumption, the initial concentration of the compound in the contaminated region is uniform throughout that region, is also accomplished after Days 81 and 123. The sediments are uniform within the analytical measurements, and in the deeper sediments, the concentration varies in the vertical direction only. Therefore, the RECOVERY simulations will start, time = 0, at Day 81 for DDE and Day 123 for lindane.

Initial water concentration for lindane was set to 25.4 and 3.5 ppt for DDE. The initial sediment concentration was set to 35.3 ppb for DDE and 1.87 ppb for lindane. Within the analytical precision of the data and the collection scheme, the above values seem to be representative of the initial conditions for the quarry exposure. The inflow to the quarry was estimated to be insignificant in comparison to the overall volume of water in the quarry (Di Toro and Paquin 1983). The water depth in the quarry was 13.9 m, and the quarry contained 5.23×10^7 l of water (Waybrant 1973).

The depth of the mixed sediment layer was set to 1.0 cm for DDE and 3.0 for lindane since DDE was not detected at substantial levels below 1.5 cm. In this case, the depth of the deep contaminated sediments was set to the allowable minimum, which was 0.05 m (0.06 m for the lindane run) below which RECOVERY can become unstable. Suspended solids were set to 5 mg/l based on an analysis by Di Toro and Paquin (1983) on Secchi disc readings and sediment trap data. Resuspension was set to zero, the burial velocity was set to 5.0×10^{-4} m/year, and the settling velocity was estimated from the solids mass balance in RECOVERY. The estimated value was 87.5 m/year; both the settling velocity and the burial velocity are within the range reported by Chapra (1983).

The partition coefficient for DDE was computed as 154,000 l/kg based on an assumed organic content of 0.05 (weight fraction) and an octanol/water partition coefficient of 5×10^4 (mg/m³ octanol)/(mg/m³ water). The molecular diffusivity was set to the default of 5×10^{-6} cm²/sec, the calculated volatilization rate for DDE was 5.09 per year, and the degradation rate was set to zero for DDE (half-life of 15 years (Howard et al. 1991)).

For lindane, the volatilization rate was 6.62×10^{-2} per year, and the degradation rate was set to 0.9 per year in both the water column and the sediments. The degradation rate agrees with the value of 0.0025/day used by Di Toro and Paquin (1983) in their application. A detailed listing of the input data for both the lindane and DDE runs is included in Appendix B.

Simulation Results

The physical and chemical parameters estimated and selected in the previous section were used in the simulation of DDE and lindane in a flooded limestone quarry. Results from the initial experiment and follow-up work were used to compare with the simulation from RECOVERY.

The simulated and observed lindane distributions are shown in Figures 3 and 4 for water and bottom sediments. Lindane decreases from 25 ppt to less than 1 ppt after 5 years in the water column. Lindane in the sediment decreases from 1.87 ppb to below 1 ppb after 5 years. Figure 5 shows the volatilization of lindane from the water column, a mechanism in the depuration of lindane from the water column. Lindane's degradation (0.9/year) is the major mechanism for the decrease from the water and thus the flux from the sediments back into the water column (Figure 6).

Figures 7 and 8 show the DDE concentration in the water column and sediment bed, respectively. A major removal mechanism for DDE is volatilization from the water column as shown in Figure 9. Initially, DDE was transferred to the sediment bed by deposition of suspended sediment contaminated with DDE from the quarry initial application. After the initial loading to the bed,

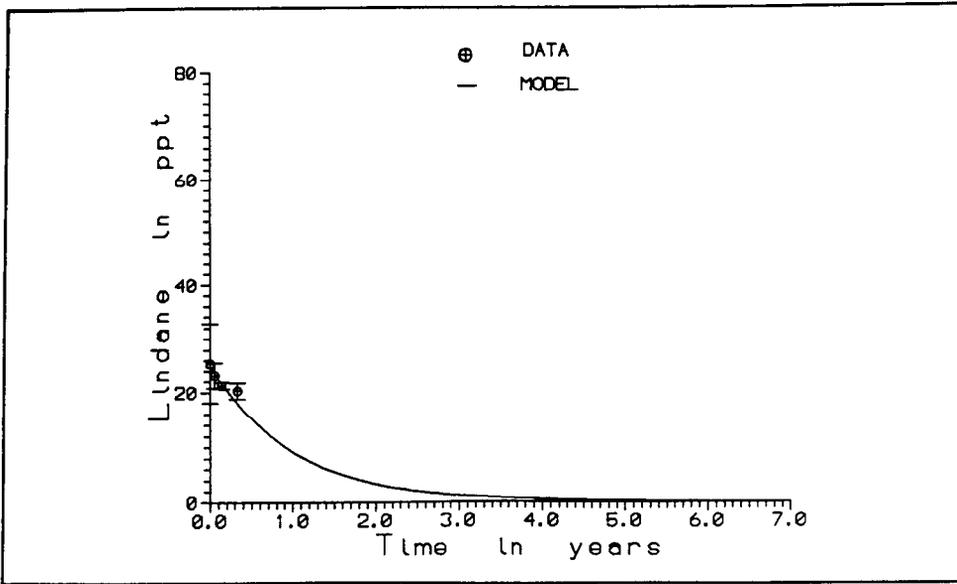


Figure 3. Lindane in water column

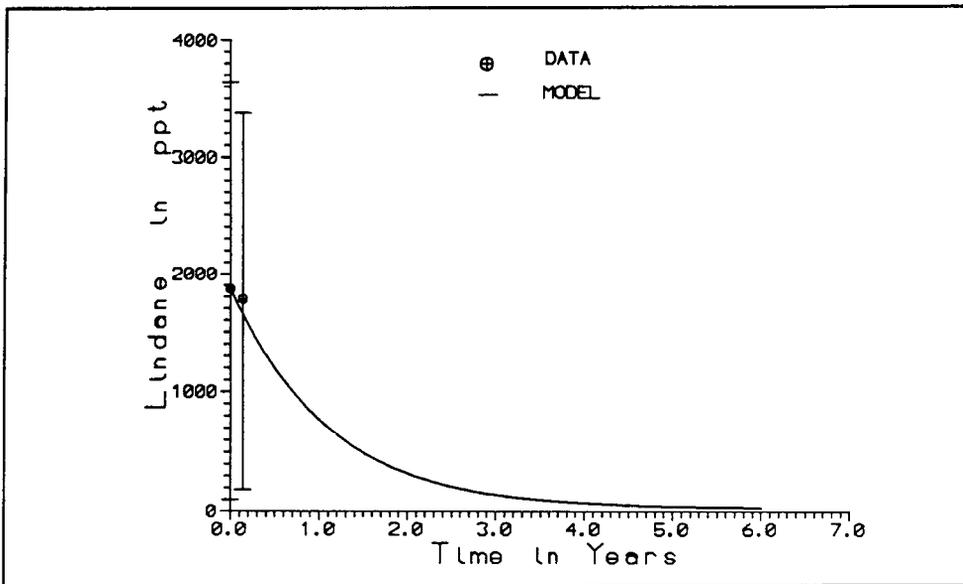


Figure 4. Lindane in sediment

the process reverses once the water column concentration starts decreasing because of the loss of DDE by volatilization. At this point, the sediment bed becomes the source of DDE for the water column (time = 0, see Figure 10) since there is no degradation in the bed; the only removal mechanism is volatilization. Contrary to lindane, where the pesticide was mostly in the water column, DDE is mostly in the bed; thus, it takes longer to clean the bed than it does to clean the water. If degradation in the sediment bed was significant, then a much faster cleanup would occur.

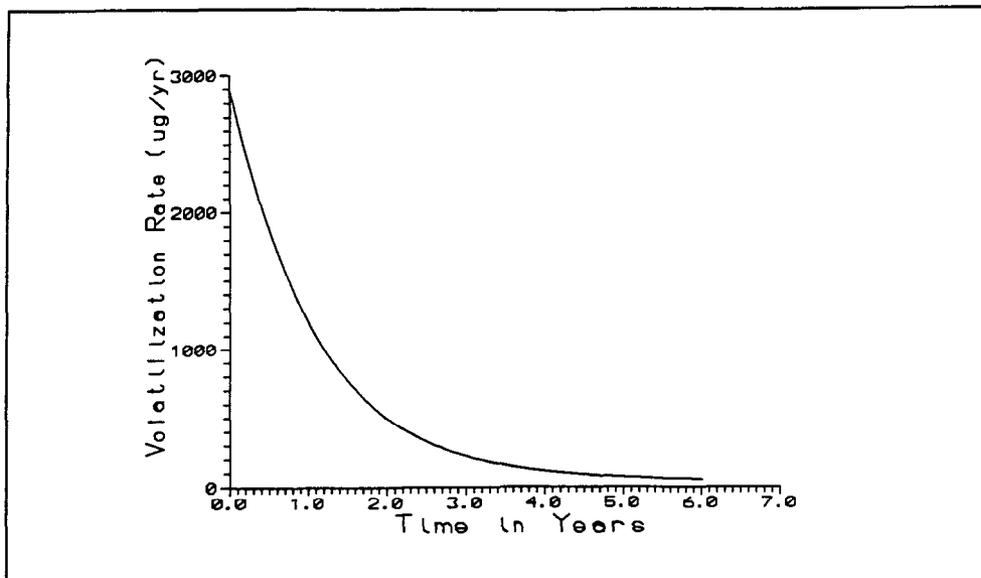


Figure 5. Volatilization rate of lindane from water computed by model

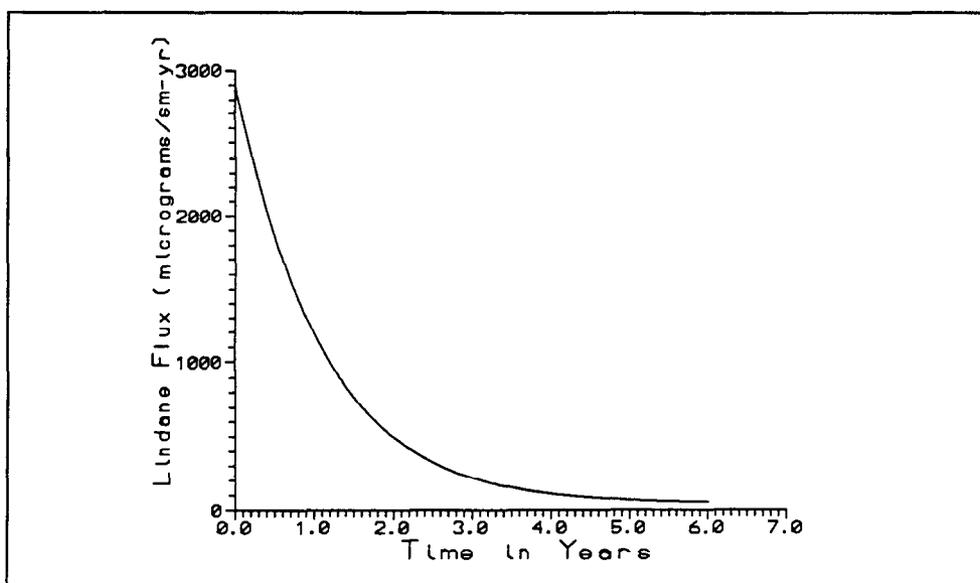


Figure 6. Flux of lindane from sediments into water computed by model

DDE in the water column after 5 years agrees very well with Di Toro's (Di Toro and Paquin 1983) prediction of less than 1 ppt (Figure 7). In the sediment, the simulation (Figure 8) shows agreement with the field data, but a little higher than the Di Toro's result of 5.6 ppb (Di Toro and Paquin 1983). However, both models predict a sediment concentration after 10 years of approximately 1 ppb. Figures 11 and 12 present a second simulation of DDE in the water and sediment bed, respectively. Porosity in the mixed bed was increased to 0.8, and the degradation of DDE in the water was set to 3.0 per

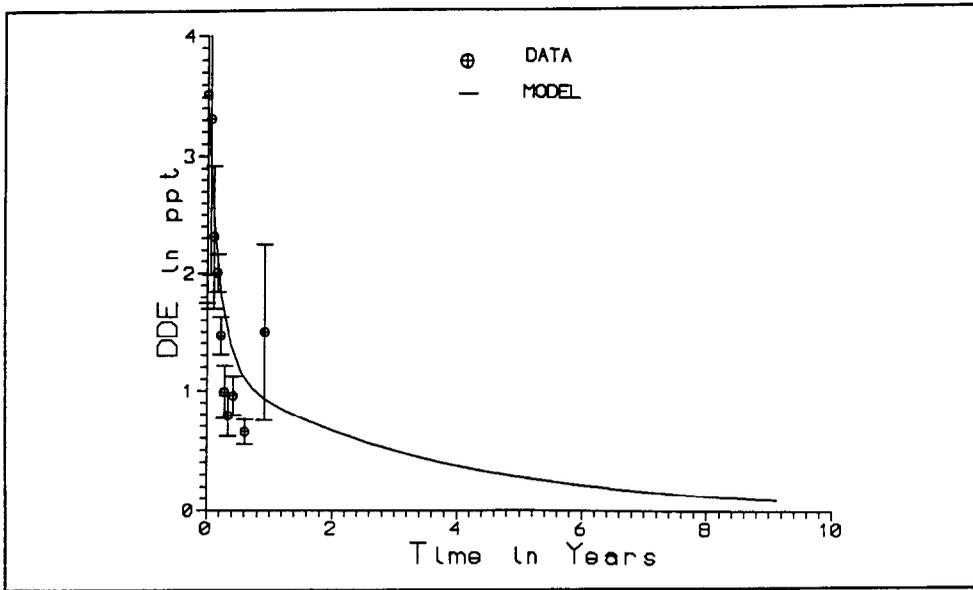


Figure 7. DDE in water column

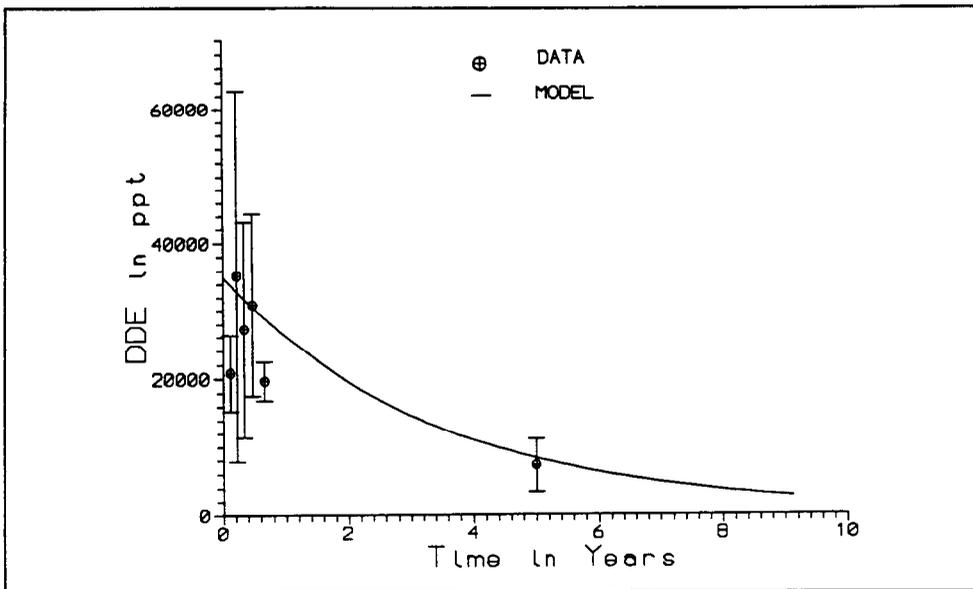


Figure 8. DDE in sediment

year to account for photodegradation of DDE. The value of 3.0/year is similar to the one used by Di Toro, 0.013/day (4.75/year) (Di Toro and Paquin 1983). This simulation agrees more closely with the other model results and shows remarkable agreement with the field data with the exception of spring sampling.

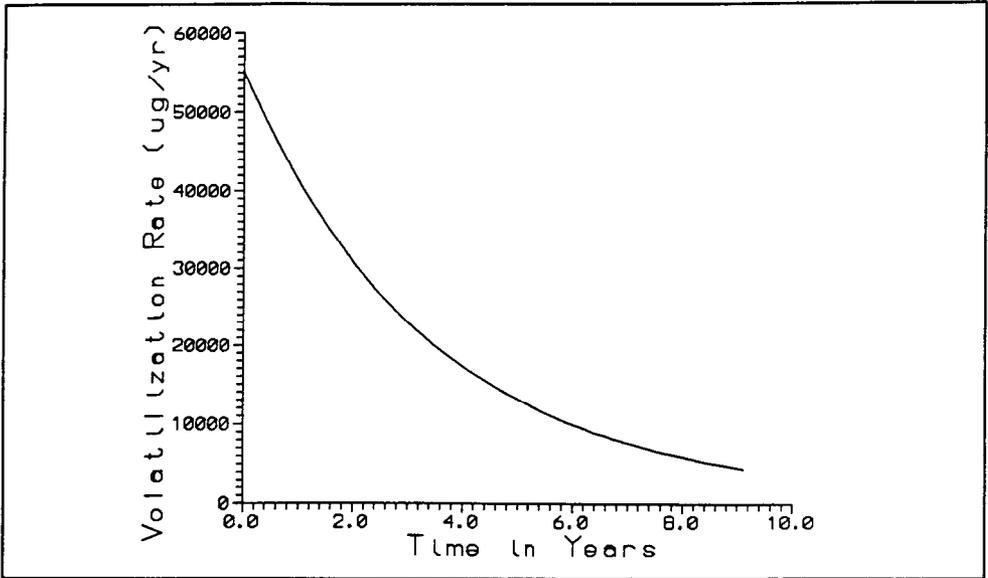


Figure 9. Volatilization rate of DDE from water computed by model

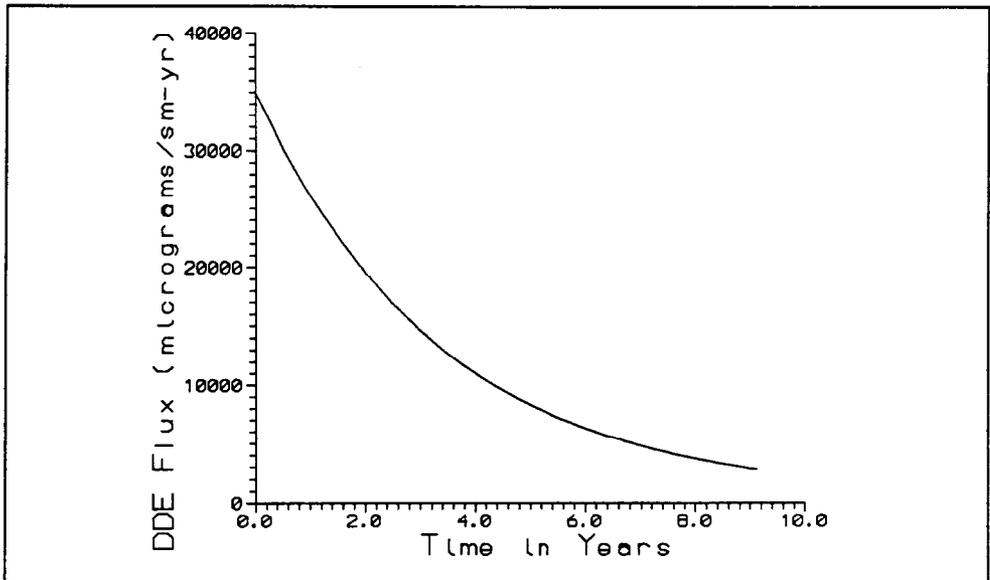


Figure 10. Flux of DDE from sediments into water computed by model

Overall, the simulation of DDE and lindane in the flooded limestone quarry can be simulated with confidence using the model RECOVERY. The confirmation application was performed with minimum calibration. In addition, very little data was needed to accomplish the task. There are three very important advantages of the RECOVERY model: the ease of application, the flexibility of the input data requirements, and the user friendly environment of the model.

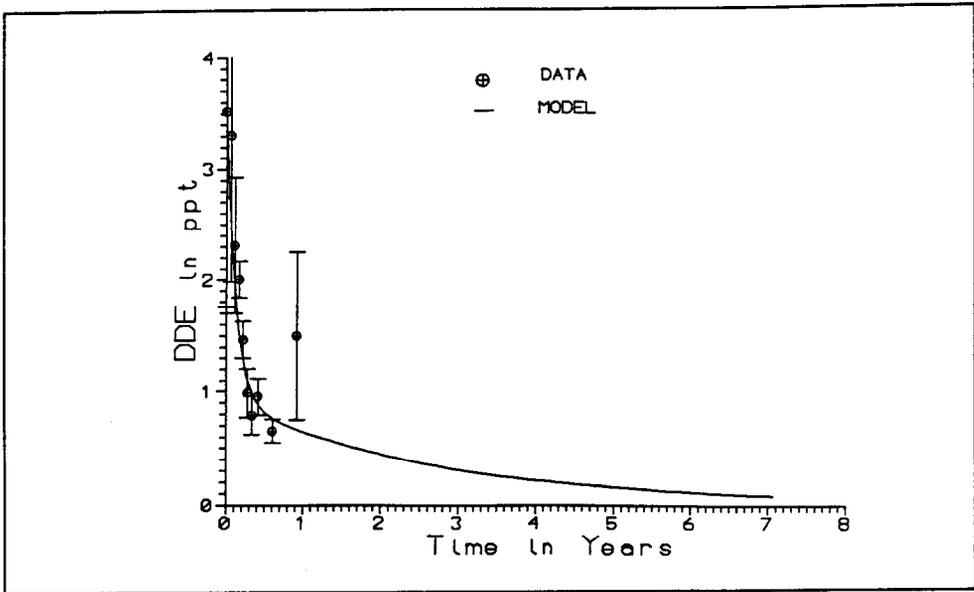


Figure 11. Final simulation of DDE in water column

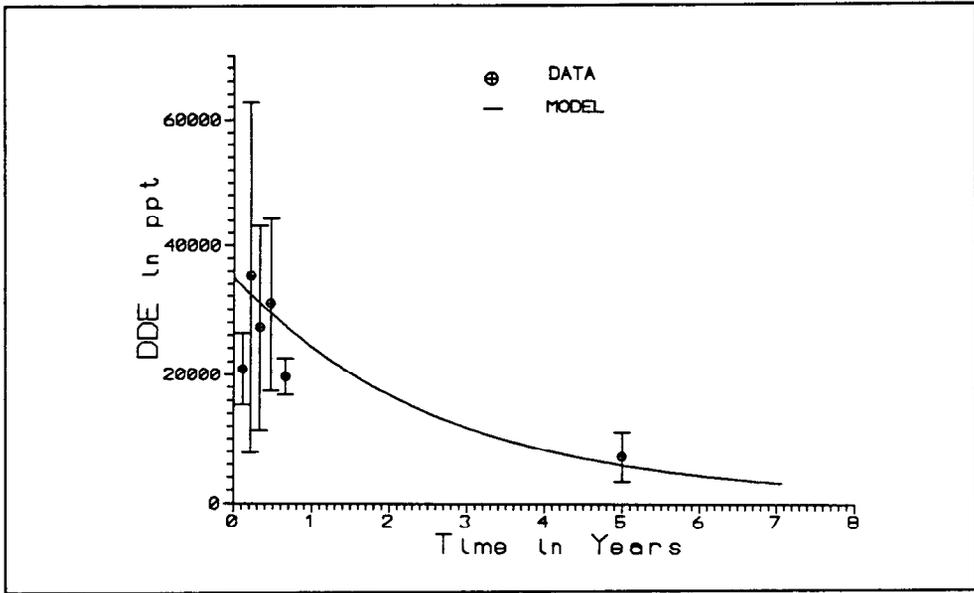


Figure 12. Final simulation of DDE in sediment

4 User's Guide

Use of the RECOVERY program is described in this section. Two files are required to run this program-RECOVERY.EXE and CORPCOMP.DAT. CORPCOMP.DAT contains the chemical database information. The other files included on the distribution disk are only required for specific hardware systems and to alter the database. (See Changing Chemical Database and System Specific Issues below.) Source code for the model is also included. (See Model Source). Do not run RECOVERY from a write-protected disk, as this will result in an error.

To start the program, move to the directory that contains the software and type RECOVERY at the DOS prompt. The first screen is a title screen. Press ENTER to view the introduction screen, which follows. Press ENTER again, and choose between creating a new file and retrieving data from an existing data file. If the second selection is made, any files ending in .REC and the subdirectories located in the current directory are displayed. The .REC files are the data files that are created when saving a run made by RECOVERY. (This will be discussed later). If your file is not located in the current directory or in one of the listed subdirectories, press BACKSPACE and specify the path name to your file. Your REC file should then be displayed. After a file is chosen, you can either view and/or change the input file or just run the model using that data file. If "create a new file" is chosen, a list of compounds is displayed. The properties of 18 compounds are included in the database. If the compound under consideration is not listed, choose number 0. The selection is made by moving the cursor to the desired selection using the arrow keys and pressing ENTER.

If selection 0 was made, a screen appears to enter the name of the contaminant. As the user types, the name will appear in the highlighted area. Corrections can be made by using the BACKSPACE or DELETE keys. After the name has been typed in, press ENTER to enter the name. If changes are necessary at this point, pressing F2 will allow modification of the name. If the user starts to type without pressing F2, the first entry is lost and the new name appears. This editing process is similar to that used by Lotus 1-2-3 (R) and is used on all input screens. Press F10 to store the data and advance to the next screen.

The next five screens are used to enter or change input values. After typing in a cell, the user must press ENTER before proceeding to the next cell. The first morphometry and hydrology screen should be displayed. If a different compound is desired at this point, pressing ESCAPE will allow this change. The user may change or leave the water concentration at the default value of zero. Three of the next four values need to be entered. Press F9 to calculate the fourth, and its values will be displayed. When all the data is entered, press F10 to store the values and advance to the next screen. If invalid values are entered, a message will appear at the bottom of the screen.

The next screen is for the contaminated sediments layer. If nothing is changed, the default values will be used. Press F10 to continue. System properties are listed on the next screen. Default values are listed for the first eight variables. These values can be changed as described above. Since the three velocity values are interrelated, two of the three values need to be entered. Typical values are listed in the center column. After entering two values, press F9 to calculate the third value. It will appear near the bottom of the screen. Press F10 to store the data and proceed.

The next two screens list contaminant properties. Default values are listed in the far right column and will be specific to the selected compound if it is in the database. These values will be used unless the user changed them in the center column. The second screen also contains intermediate values calculated from the previously entered data (e.g., F_{dw} and K_{dw}). Press F10 to store and advance.

If the user wants to return to a previous screen in the input process described above, he/she can press ESCAPE until the desired screen appears.

The next screen serves as a check to see if the entered data are correct; if not, the user can return to the input screens. Selecting the third option starts the model. If graphics capabilities are available on the system being used, the concentration profile in the deep sediments is displayed. The total number of years is calculated as the approximate time when the water concentration decreases to 10 percent of its maximum value. Since the numerical method uses an adaptive-step-size, the time between profile displays will not be even. When the computation is finished, a message appears in the lower right-hand corner of the screen.

After a key is pressed, another menu appears. If one of the first five options is chosen or number 8, this menu appears again so another selection can be made. Options 1-4 are graphics plots. If the system being used does not have graphics capabilities, a message appears informing the user of this, and a key can be pressed to return to the menu. Results on systems having graphics capabilities other than those listed in Chapter 4 of this report will be unpredictable. The first two plots are graphs of the contaminant concentration in the water layer and the mixed layer, respectively, versus time. The third plot shows the flux of the contaminant from the sediments to the water versus time. A graph of the volatilization rate of the contaminant will be displayed if

number 4 is selected. These results can be printed by typing Shift + Print Screen. Select number 5 to print a table of results on the printer. Number 6 should be selected to make modifications to the existing run, and number 7 should be used to return to the beginning of the program. Choose number 8 to save the existing run. The user will be prompted for a file name to be used to store the results. Choosing number 9 will result in exiting the program.

Changing Chemical Database

Currently, data for 18 chemicals are included in the data file, CORPCOMP.DATA. This file can be changed and enlarged to include a maximum of 39 compounds. Changes are made by altering the file CORPSDAT.BAS, which is included with the distribution disk. This file contains the following data for a compound:

Name
Molecular Weight
Octanol-Water Partition Coefficient
Henry's Constant
Molecular Diffusivity
Decay Constants--water, dissolved phase
 water, particulate phase
 mixed layer, dissolved phase
 mixed layer, particulate phase
 deep sediments, dissolved phase
 deep sediments, particulate phase

Additions and changes are made by altering or adding data statements to the file CORPSDAT.BAS and running the program. Errors will occur in RECOVERY if there are more than 39 compounds, a compound name with greater than 28 letters, or additional parameters are added to the data statements.

Model Source

In order to access the model source code in the QuickBasic environment, type qb recovery /I replib when you are in a directory containing QuickBasic Version 4.5 and the following files (included on the distribution disk):

RECOVERY.MAK
RECOVERY.BAS
CRANK.BAS
ADAPTEST.BAS
MODEL.BAS
RECLIB.QLB

Program Features

A list of data needed to run this program can be found in Table 4. Since the compound properties for several contaminants are included in the provided database, the user needs to provide compound properties only if the contaminant under consideration is not one that is in the database. The values in the database that comes with the distribution disk are listed in Table 5. The data file can be changed as described in Chapter 5.

The data are entered on a series of input screens with editing capabilities. The user can easily page forward and backward through the screens while entering data. On-line help is also available. If any of the entered data are invalid, an error message appears instructing the user to re-enter the data. For computers with graphic display capabilities, the deep-sediment concentration profile will be displayed during the model computation.

Table 4
Input Data for RECOVERY Model

Water Column Morphometry/Hydrology (3 specified, 4th computed)

Flow through, m^3/year
 Residence time, year
 Surface area, m^2
 Water depth, m

Water Layer:

Initial concentration, $\mu\text{g}/\text{m}^3$

Contaminated Sediments:

Depth of contaminated sediment layer, m
 Depth of mixed layer, m
 Mixed layer surface area, m^2
 Initial concentrations, $\mu\text{g}/\text{m}^3$
 Mixed layer
 Deep contaminated sediments

System Properties:

Suspended solids concentration in water, g/m^3
 Mixed layer porosity
 Deep sediment porosity
 Sediment particle density, g/m^3
 Wind speed, m/s
 Fraction organic carbon, **g-orgC/g-dry** wt solids
 Water layer
 Mixed layer
 Deep contaminated sediments

Two of the following three velocities:
 Resuspension velocity, m/s
 Burial velocity, m/s
 Settling velocity, **m/s**

Compound Properties:

Molecular diffusivity, cm^2/s
 Decay coefficients, per year: particulate - water
 dissolved - water
 particulate - mixed layer
 dissolved - mixed layer
 particulate - deep sediments
 dissolved - deep sediments

Henry's constant, $\text{atm}\cdot\text{m}^3/\text{gmole}$
 Octanol-water partition coefficient
 Molecular weight, g/gmole

Table 5 Compound Properties			
Compound	Henry's Constant @ 25 °C atm m³/gmole	log (<i>K_{ow}</i>)	Molecular Weight g/gmole
Chlordane	4.8 × 10 ⁻⁵	2.78	409.6
DDT	3.9 × 10 ⁻⁵	5.00	354.5
Dieldrin	2.0 × 10 ⁻⁷	3.54	381.0
Lindane	4.9 × 10 ⁻⁷	3.70	290.0
Arochlor 1242	8.4 × 10 ⁻³	6.72	328.4
Arochlor 1248	3.5 × 10 ⁻³	6.00	295.0
Arochlor 1254	2.8 × 10 ⁻³	6.00	326.0
Arochlor 1260	7.1 × 10 ⁻³	6.50	361.0
Benzene	5.5 × 10 ⁻³	2.10	78.0
Chlorobenzene	3.7 × 10 ⁻³	2.98	112.6
Ethylbenzene	8.7 × 10 ⁻³	3.15	106.0
Pentachlorophenol	3.4 × 10 ⁻⁶	5.00	266.0
Phenol	1.3 × 10 ⁻⁶	1.46	94.1
Toluene	6.7 × 10 ⁻³	2.70	92.0
Anthracene	1.7 × 10 ⁻³	4.45	178.2
Benzo(a)pyrene	7.2 × 10 ⁻⁷	5.00	252.0
Naphthalene	4.3 × 10 ⁻⁴	3.36	128.0
Chloroform	4.2 × 10 ⁻³	1.95	119.0
Note: Values for Henry's constant <i>K_{ow}</i> and molecular weight are from Lyman et al. (1982), Schnoor et al. (1987) and Thomann and Mueller (1987). The default values for all molecular diffusivities are 5 × 10 ⁻⁶ cm ² /s. The default values for all decay coefficients are zero.			

The final results are displayed as plots on the screen and can be printed on a printer using the Shift+Print Screen command. Numerical results can be dumped to the printer also. The plots are as follows:

- a. Contaminant concentration in the water versus time.
- b. Contaminant concentration in the mixed layer versus time.
- c. Flux of the contaminant from the sediments into the water versus time.
- d. Volatilization losses of the contaminant from the water versus time.

The input data can be stored on a disk and retrieved for later use. The user can also easily return to the input screens to make modifications. Appendix C gives a sequential example of the screens in running the RECOVERY model.

This program is written in Microsoft QuickBASIC 4.5 and has been written for the following combinations of graphic adapters and displays:

CGA and Color Display
EGA and Monochrome Display
EGA and Color Display
EGA and Enhanced Color Display
VGA and Monochrome Display
VGA and Color Display
Hercules Video Card and Monochrome Display

A math coprocessor is not required to run RECOVERY. The use of one, however, will decrease the computation time.

System Specific Issues

The following list describes some procedures that are specific to particular hardware systems. If you have problems running RECOVERY, please consult the list below.

a. Use of Hercules Graphics Card

If your system has a Hercules Graphics Card, you will need to load the Hercules driver before running the program. The driver, MSHERC.COM, ((C) Copyright Microsoft Corporation, 1987, 1988) is provided on the distribution disk. To run the program, type MSHERC. If you do not nm this program, the model should run but not display any graphics.

b. Strange Sediment Profile Results

If your system has all of the following characteristics, you may have floating-point math problems.

- Uses MS-DOS Version 3.20.
- Boots from a hard drive.
- Has a math coprocessor (for instance, an 8087 chip).

These problems can be avoided by booting the computer from a floppy disk drive instead of the hard drive.

WARNING: If you have floating-point math problems, the model information will not be correct. This should be evident by the graphical results.

c. Use of a Compaq 386 with a Math Coprocessor

If you are using a Compaq 386 that has a math coprocessor installed, RECOVERY may crash. In order to use the model, turn the coprocessor off by adding the line SET NO87 = '' to the CONFIG.SYS file and rebooting your machine.

5 Conclusions and Recommendations

RECOVERY is designed for interactive implementation via a personal computer. The program allows the user to rapidly generate and analyze recovery scenarios for contaminated sediments. The software includes graphical displays and is self-documented. The intent of this report is to document the model and confirm it against existing field data.

The confirmation of RECOVERY against the quarry experiments shows the ability of the program to simulate behavior of organics in a real system with a limited amount of data. Results are similar to those predicted by another model and, thus, appear to demonstrate the validity of the algorithms used to describe the fate and transport of organics.

One problem found in the confirmation exercise was the simulation of the initial part of the quarry experiment where an initial organic load was applied to the pond. The current formulation of the model assumes no loadings associated with the inflow. To overcome the loading problem and the completely mixed assumption, the simulation was started at a time where the sediments were contaminated with pesticides, and the surface water pesticide concentration was fairly uniform throughout the pond. After satisfying the model assumptions, the simulation proceeded with good results when compared with both the data collected at the site and another model.

The RECOVERY model can be applied in a variety of scenarios, including lakes, embayments, harbors, estuaries, and ocean parcels, as long as the assumptions of a completely mixed water body is acceptable along with other assumptions listed in Table 1. Average yearly flushing would be needed in any of the applications above, in addition to the other chemical and physical parameters for a well-defined simulation.

Mechanistic and/or modular improvements recommended for RECOVERY are the following:

- a.** Allow external contaminant loadings from point and nonpoint sources.
- b.** Allow atmospheric contaminant loads, such as dry or wet deposition.

- c. Allow the variation of physical and chemical properties in the contaminated sediment.
- d. Include food chain uptake, such as fish gill exchange and sediment uptake.
- e. Develop a version of RECOVERY to assess the impact on surface waters from bottom sediments contaminated with heavy metals.

The above recommendations include both short-term modifications (the first two) and long-term improvements. The short-term modifications will provide a wider range of applications for the RECOVERY model and would not be major modifications of the program. Recommendations c and d are a major undertaking and would imply substantial modifications of the program. The last recommendation would involve substantial effort since both transport and kinetic algorithms would need modifications and/or development.

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Appendix A

Nomenclature

A_m	Mixed layer surface area, m^2 .
A_w	Water surface area, m^2 .
C_i	Contaminant concentration in the inlet to the water body, $\mu g/m^3$.
C_m	Contaminant concentration in the mixed layer, $\mu g/m^3$.
C_{m0}	Initial contaminant concentration in the mixed layer, $\mu g/m^3$.
C_s	Contaminant concentration in the deep sediments, $\mu g/m^3$.
C_{s0}	Initial contaminant concentration in the deep sediments, $\mu g/m^3$.
$C_{s(O)}$	Contaminant concentration at the top of the deep sediments, $\mu g/m^3$.
C_w	Contaminant concentration in the water, $\mu g/m^3$.
C_{w0}	Initial contaminant concentration in the water, $\mu g/m^3$.
D_s	Molecular diffusivity, m^2/s .
D_m	Diffusion coefficient in the sediment pore water, m^2/s .
F_{dpm}	Ratio of contaminant concentration in the mixed layer pore water to concentration in the total mixed layer, dimensionless.
F_{dps}	Ratio of contaminant concentration in the deep sediment pore water to concentration in the total deep sediments, dimensionless.
F_{dw}	Fraction of contaminant in particulate form in the water, dimensionless.

f_{oc}	Weight fraction of organic carbon in the solid matter, g-orgC/g-solid.
F_{pw}	Fraction of contaminant in dissolved form in the water, dimensionless.
H_e	Henry's law constant, dimensionless.
H_e'	Henry's law constant, atm-m ³ /gmole.
J	Flux of the contaminant, g/(m ² -year).
J_{ms}	Flux of the contaminant from the mixed layer to the deep sediments, g/(m ² -year).
K_{dw}	Contaminant partition coefficient in the water, m ³ /g.
K_{ds}	Contaminant partition coefficient in the sediments, m ³ /g.
K_g	Gas-film mass transfer coefficient, m/year.
K_l	Liquid-film mass transfer coefficient, m/year.
k_m	Decay rate constant of the contaminant in the mixed layer, /year.
K_{ow}	Octanol-water partition coefficient, (mg/m ³ -Octanol)/(mg/m ³ -water).
k_s	Decay rate constant of the contaminant in the deep sediments, /year.
k_v	Volatilization rate of the contaminant, /year.
k_w	Decay rate constant of the contaminant in the water, /year.
MW	Molecular weight of the contaminant, g/gmole.
Q	Flow rate into and out of the water body, m ³ .
R	Universal gas constant, atm-m ³ /(gmole-kelvins).
s_w	Suspended solids concentration in the water, g/m ³ .
t	Time, years.
T	Absolute temperature, kelvins.
v_b	Burial velocity, m/year.

v_d	Diffusive mass transfer coefficient, m/year.
V_m	Volume of the mixed layer, $\mathbf{m^3}$.
v_r	Resuspension velocity of the sediments into the water, m/year.
v_s	Settling velocity of the particulate matter from the water to the sediments, m/year.
v_v	Volatilization transfer coefficient, m/year.
V_w	Volume of the water, $\mathbf{m^3}$.
U_w	Wind speed, m/year.
z'	Length over which the concentration gradient exists at the sediment/water interface, m.
z_m	Depth of the mixed layer, m.
z_w	Depth of the water layer, m.
ρ	Density of the sediment solids, $\mathbf{g/m^3}$.
ϕ	Porosity

Appendix B

Input Screens for DDE and Lindane Runs

RECOVERY RUN DDE

MORPHOMETRY AND HYDROLOGY

Water

Mixed

Deep Contaminated Sediments

Clean Sediments

WATER

Initial Concentration of DDT ($\mu\text{g}/\text{m}^3$): 3.500E+00

ENTER 3 OF THE FOLLOWING 4 VALUES AND PRESS F9:

Water Surface Area (m^2):	1000E+00
Water Depth (m):	10.0
Flow Through (m^3/yr):	
Residence Time (years):	50.00

Calculated Flow Through (m^3/yr): 200.00

Help-F1 Edit-F2 ReCalc-F9 Store Data/Advance-F10 Change Compound-Esc

INPUT SCREEN 1

MORPHOMETRY AND HYDROLOGY

Water

Mixed

Deep Contaminated Sediments

Clean Sediments

CONTAMINATED SEDIMENTS LAYER

L = Contaminated Sediment Depth (m): 0.05

z = Depth of Mixed Layer (cm): 1.00

Mixed Layer Surface Area (m^2): 1000E+00

Initial Concentrations ($\mu\text{g}/\text{m}^3$)

Mixed Layer:	3.500E+04
Deep Contaminated Sediments:	3.500E+04

Help-F1 Edit-F2 Store Data and Advance-F10

INPUT SCREEN 2

RECOVERY RUN
DDE

SYSTEM PROPERTIES		
Suspended Solids Concentration in Water (g/n ³):		5.00
Mixed Sediment Porosity:		0.65
Deep Sediment Porosity:		0.65
Mixed Sediment Particle Density (g/n ³):		2.50E+06
Deep Sediment Particle Density (g/n ³):		2.50E+06
Wind Speed (m/sec):		2.00
Weight fraction carbon in solid - water:		5.00E-02
Weight fraction carbon in solid - mixed layer:		5.00E-02
Weight fraction carbon in solid - sediments:		5.00E-02
INPUT TWO OF THE FOLLOWING VELOCITIES AND PRESS F9:		
Velocity (m/yr)	Typical Value	Value for this Run
Resuspension Velocity:	0.00E+00	0.00E+00
Burial Velocity:	5.34E-04	5.00E-04
Settling Velocity:	1.00E+02	
Calculated Settling Velocity (m/yr):		0.75E+01
Help-F1 Edit-F2 ReCalc-F9 Store Data and Advance-F10		

INPUT SCREEN 3

DDT PROPERTIES		
Property	Value for This Run	Default Value
Henry's Con. (atm-n ³ /gmole)	3.90E-05	3.90E-05
Molecular Weight	354.50	354.50
Octanol-Water Partition Coeff. (mg/n ³ octanol)/(mg/n ³ water)	5.00E+04	5.00E+04
CALCULATED DATA		
F _{dw}	9.92E-01	9.92E-01
F _{pw}	7.65E-03	7.65E-03
F _{dpw}	1.73E-03	1.73E-03
F _{dps}	7.41E-04	7.41E-04
Partition Coefficients:		
K _{dw}	1.54E-03	1.54E-03
K _{dn}	1.54E-03	1.54E-03
K _{ds}	1.54E-03	1.54E-03
Volatilization rate (1/yr)	5.09E+00	5.09E+00
Help-F1 Edit-F2 ReCalc-F9 Store Data and Advance-F10		

INPUT SCREEN 4

RECOVERY RUN2
DDE

MORPHOMETRY AND HYDROLOGY

WATER

Initial Concentration of DDT ($\mu\text{g}/\text{m}^3$): **3.500E+00**

ENTER 3 OF THE FOLLOWING 4 VALUES AND PRESS F9:

Water Surface Area (m^2): 1000E+00
 Water Depth (m): 10.0
 Flow Through (m^3/yr):
 Residence Time (years): 50.00

Calculated Flow Through (m^3/yr): 200.00

Help-F1 Edit-F2 ReCalc-F9 Store Data/Advance-F10 Change Compound-Esc

INPUT SCREEN 1

MORPHOMETRY AND HYDROLOGY

CONTAMINATED SEDIMENTS LAYER

L = Contaminated Sediment Depth (m): **0.05**
 z = Depth of Mixed Layer (cm): 1.00
 Mixed Layer Surface Area (m^2): 1000E+00

Initial Concentrations ($\mu\text{g}/\text{m}^3$)
 Mixed Layer: 3.500E+04
 Deep Contaminated Sediments: 3.500E+04

Help-F1 Edit-F2 Store Data and Advance-F10

INPUT SCREEN 2

RECOVERY RUN2
DDE

SYSTEM PROPERTIES		
Suspended Solids Concentration in Water (g/m ³):		5.00
Mixed Sediment Porosity:		0.80
Deep Sediment Porosity:		0.65
Mixed Sediment Particle Density (g/m ³):		2.50E+06
Deep Sediment Particle Density (g/m ³):		2.50E+06
Wind Speed (m/sec):		2.00
Weight fraction carbon in solid - water:		5.00E-02
Weight fraction carbon in solid - mixed layer:		5.00E-02
Weight fraction carbon in solid - sediments:		5.00E-02
INPUT TWO OF THE FOLLOWING VELOCITIES AND PRESS F9:		
Velocity (m/yr)	Typical Value	Value for this Run
Resuspension Velocity:	0.00E+00	0.00E+00
Burial Velocity:	5.34E-04	5.00E-04
Settling Velocity:	1.00E+02	
Calculated Settling Velocity (m/yr):		0.75E+01
Help-F1 Edit-F2 ReCalc-F9 Store Data and Advance-F10		

INPUT SCREEN 3

DDT PROPERTIES		
Property	Value for This Run	Default Value
Molecular Diffusivity (cm ² /sec)	1.0E-05	1.0E-05
DECAY COEFFICIENTS (1/yr)		
Dissolved Contaminant:		
In Water	3.000	0.010
In Mixed Layer	0.000	0.010
In Deep Sediments	0.000	0.010
Particulate Contaminant:		
In Water	0.000	0.010
In Mixed Layer	0.000	0.010
In Deep Sediments	0.000	0.010
Help-F1 Edit-F2 Store Data and Advance-F10		

INPUT SCREEN 4

RECOVERY RUN2
DDE

DDT PROPERTIES		
Property	Value for This Run	Default Value
Henry's Con. (atm ⁻³ /gmole)	3.98E-05	3.98E-05
Molecular Weight	354.58	354.58
Octanol-Water Partition Coeff. (mg/m ³ octanol)/(mg/m ³ water)	5.88E+04	5.88E+04
CALCULATED DATA		
F _{dw}	9.92E-01	9.92E-01
F _{pw}	7.65E-03	7.65E-03
F _{dpw}	1.38E-03	1.38E-03
F _{dps}	7.41E-04	7.41E-04
Partition Coefficients:		
K _{dw}	1.54E-03	1.54E-03
K _{dpw}	1.54E-03	1.54E-03
K _{dps}	1.54E-03	1.54E-03
Volatilization rate (1/yr)	5.89E+00	5.89E+00
Help-F1 Edit-F2 ReCalc-F9 Store Data and Advance-F10		

INPUT SCREEN 5

RECOVERY RUN
LINDANE

MORPHOMETRY AND HYDROLOGY

WATER

Initial Concentration of Lindane ($\mu\text{g}/\text{m}^3$): **2.500E+01**

ENTER 3 OF THE FOLLOWING 4 VALUES AND PRESS F9:

Water Surface Area (m^2): 1800E+00
 Water Depth (m): 18.8
 Flow Through (m^3/yr):
 Residence Time (years): 58.88

Calculated Flow Through (m^3/yr): 288.88

Help-F1 Edit-F2 ReCalc-F9 Store Data/Advance-F18 Change Compound-Esc

INPUT SCREEN 1

MORPHOMETRY AND HYDROLOGY

CONTAMINATED SEDIMENTS LAYER

L = Contaminated Sediment Depth (m): **0.136**
 z = Depth of Mixed Layer (cm): 3.00
 Mixed Layer Surface Area (m^2): 1800E+00

Initial Concentrations ($\mu\text{g}/\text{m}^3$)
 Mixed Layer: 1.878E+03
 Deep Contaminated Sediments: 2.488E+03

Help-F1 Edit-F2 Store Data and Advance-F18

INPUT SCREEN 2

RECOVERY RUN
LINDANE

SYSTEM PROPERTIES		
Suspended Solids Concentration in Water (g/m ³):		5.00
Mixed Sediment Porosity:		0.65
Deep Sediment Porosity:		0.65
Mixed Sediment Particle Density (g/m ³):		2.50E+06
Deep Sediment Particle Density (g/m ³):		2.50E+06
Wind Speed (m/sec):		1.04
Weight fraction carbon in solid - water:		5.00E-02
Weight fraction carbon in solid - mixed layer:		5.00E-02
Weight fraction carbon in solid - sediments:		5.00E-02
INPUT TWO OF THE FOLLOWING VELOCITIES AND PRESS F9:		
Velocity (m/yr)	Typical Value	Value for this Run
Resuspension Velocity:	0.00E+00	0.00E+00
Burial Velocity:	5.34E-04	
Settling Velocity:	1.00E+02	3.65E+01
Calculated Burial Velocity (m/yr):		2.09E-04
Help-F1 Edit-F2 ReCalc-F9 Store Data and Advance-F10		

INPUT SCREEN 3

LINDANE PROPERTIES		
Property	Value for This Run	Typical Value
Molecular Diffusivity (cm ² /sec)	5.0E-06	5.0E-06
DECAY COEFFICIENTS (1/yr)		
Dissolved Contaminant:		
In Water	0.900	0.010
In Mixed Layer	0.900	0.010
In Deep Sediments	0.900	0.010
Particulate Contaminant:		
In Water	0.000	0.010
In Mixed Layer	0.000	0.010
In Deep Sediments	0.000	0.010
Help-F1 Edit-F2 Store Data and Advance-F10		

INPUT SCREEN 4

RECOVERY RUN
LINDANE

LINDANE PROPERTIES		
Property	Value for This Run	Default Value
Henry's Con. (atm-n ³ /gmole)	4.98E-07	4.98E-07
Molecular Weight	298.08	298.08
Octanol-Water Partition Coeff. (ng/n ³ octanol)/(ng/n ³ water)	5.81E+03	5.81E+03
CALCULATED DATA		
F _{dw}	9.99E-01	9.99E-01
F _{pw}	7.72E-04	7.72E-04
F _{dpm}	7.36E-03	7.36E-03
F _{dps}	7.36E-03	7.36E-03
Partition Coefficients:		
K _{dw}	1.55E-04	1.55E-04
K _{dm}	1.55E-04	1.55E-04
K _{ds}	1.55E-04	1.55E-04
Volatilization rate (1/yr)	6.62E-02	6.62E-02
Help-F1	Edit-F2	ReCalc-F9 Store Data and Advance-F10

INPUT SCREEN 5

Appendix C Screens

RECOVERY

A Decision Support Model for Screening the Fate of In-Place
Contaminated Sediments in Aquatic Environments

June, 1989
Beta Test Version 1.0

Written for The U.S. Army Corps of Engineers
Waterways Experiment Station
and
New England Division

Written by Jean M. Boyer and Steven C. Chapra
Center for Advanced Decision Support
in Water and Environmental Systems
University of Colorado
Boulder, CO 80309-0428

MsHerc program (C) Copyright '87, '88 Microsoft Corp. All rights reserved.

Press any key to continue.

SCREEN 1

This program is a tool for screening the fate of in-place contaminated sediments in aquatic environments. It predicts the concentration of a contaminant in the water, the mixed sediment layer and in the deep sediments over time. The flux of the contaminant from the sediments into the water is also predicted. Note that the total number of years for which the model is run is determined by approximating the time required for the toxic concentration in the water to decrease to 10% of the maximum value achieved, up to a maximum of 100 years.

Please refer to the documentation accompanying this software for detailed instructions and model theory.

If you need help while entering data into an input screen, press F1. Press Ctrl-Break to terminate the program at any time. Press Shift-Print Screen to print a graph displayed on the screen.

Press any key to continue.

SCREEN 2

Highlight your choice and press Enter or
press the number preceding your selection.

1. Create a new file.
2. Retrieve data from an existing file.

SCREEN 3

These are the .REC files and subdirectories listed in the specified
directory. Highlight one of these using the up and down arrows and
press Enter or press Backspace to specify an alternative directory.
Press escape to return to the previous screen.

Directory: C:\QB45\

CHLOR.REC ANTH.REC

SCREEN 4a

The properties of the following contaminants are included in the database.
If the contaminant you want to consider is not listed, choose 0.

Highlight your choice using the arrow keys and press ENTER.

- | | |
|------------------------|-----------------------|
| 0. Compound Not Listed | 10. Chlorobenzene |
| 1. Chlordane | 11. Ethyl Benzene |
| 2. DDT | 12. Pentachlorophenol |
| 3. Dieldrin | 13. Phenol |
| 4. Lindane | 14. Toluene |
| 5. Arochlor 1242 | 15. Anthracene |
| 6. Arochlor 1248 | 16. Benzo(a)pyrene |
| 7. Arochlor 1254 | 17. Naphthalene |
| 8. Arochlor 1260 | 18. Chloroform |
| 9. Benzene | |

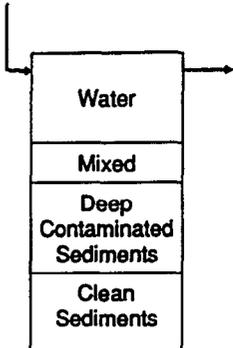
SCREEN 4b

Highlight your choice and press Enter or
press the number preceding your selection.

1. View/Change Input file.
2. Run Using Input File.

SCREEN 5

MORPHOMETRY AND HYDROLOGY



Water

Initial Concentration of Chlordane ($\mu\text{g}/\text{m}^3$): 0.000E+00

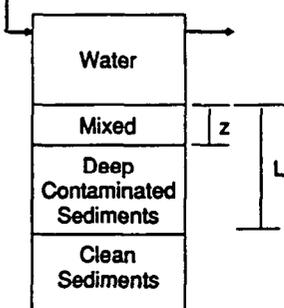
ENTER 3 OF THE FOLLOWING 4 VALUES AND PRESS F9:

Calculated Residence Time (years): 5.00

Help-F1 Edit-F2 ReCalc-F9 Store Data/Advance-F10 Change Compound-Esc

SCREEN 6

MORPHOMETRY AND HYDROLOGY



CONTAMINATED SEDIMENTS LAYER

L = Contaminated Sediment Depth (m): 1.00
z = Depth of Mixed Layer (cm): 5.00
Mixed Layer Surface Area (m^2): 1000E+04

Initial Concentrations ($\mu\text{g}/\text{m}^3$)
Mixed Layer: 1.000E+03
Deep Contaminated Sediments: 1.000E+03

Help-F1 Edit-F2 Store Data and Advance-F10

SCREEN 7

SYSTEM PROPERTIES

Suspended Solids Concentration in Water (g/m³): 2.00
 Mixed Sediment Porosity: 0.85
 Deep Sediment Porosity: 0.85
 Mixed Sediment Particle Density (g/m³): 2.50E+06
 Deep Sediment Particle Density (g/m³): 2.50E+06
 Wind Speed (m/sec): 5.00
 Weight fraction carbon in solid - water: 5.00E-02
 Weight fraction carbon in solid - mixed layer: 5.00E-02
 Weight fraction carbon in solid - sediments: 5.00E-02

INPUT TWO OF THE FOLLOWING VELOCITIES AND PRESS F9:

Velocity (m/yr)	Typical Value	Value for this Run
Resuspension Velocity:	0.00E+00	0.00E+00
Burial Velocity:	5.34E-04	5.00E-04
Settling Velocity:	1.00E+02	
Calculated Settling Velocity (m/yr):		9.37E+01

Help-F1 Edit-F2 ReCalc-F9 Store Data and Advance-F10

SCREEN 8

CHLORDANE PROPERTIES

Property	Value for This Run	Default Value
Molecular Diffusivity (cm ² /sec)	5.0E-06	5.0E-06
DECAY COEFFICIENTS (1/yr)		
Dissolved Contaminant:		
In Water	0.000	0.010
In Mixed Layer	0.000	0.010
In Deep Sediments	0.000	0.010
Particulate Contaminant:		
In Water	0.000	0.010
In Mixed Layer	0.000	0.010
In Deep Sediments	0.000	0.010

Help-F1 Edit-F2 Store Data and Advance-F10

SCREEN 9

CHLORDANE PROPERTIES

Property	Value for This Run	Default Value
Henry's Con. (atm-m ³ /gmole)	4.80E-05	4.80E-05
Molecular Weight	409.60	409.60
Octanol-Water Partition Coeff. (mg/m ³ octanol)/(mg/m ³ water)	6.03E+02	6.03E+02
CALCULATED DATA		
Fdw	1.00E+00	1.00E+00
Fpw	3.72E-05	3.72E-05
Fdpm	1.28E-01	1.28E-01
Fdps	1.28E-01	1.28E-01
Partition Coefficients		
Kdw	1.86E-05	1.86E-05
Kdm	1.86E-05	1.86E-05
Kds	1.86E-05	1.86E-05
Volatilization rate (1/yr)	1.14E+01	1.14E+01

Help-F1

Edit-F2

ReCalc-F9

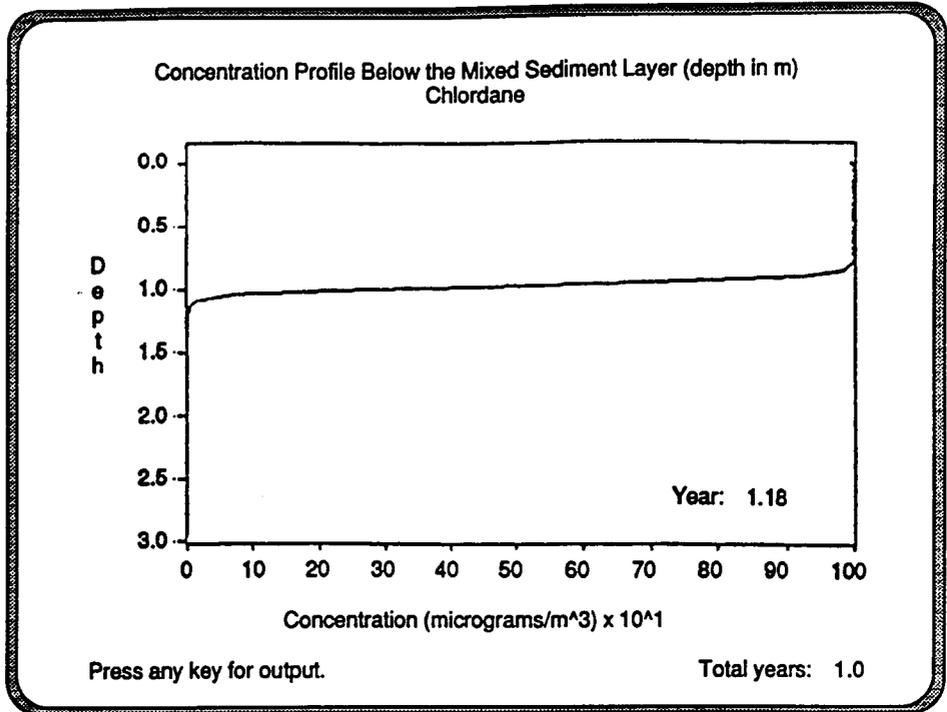
Store Data and Advance-F10

SCREEN 10

Highlight your choice and press Enter or
press the number preceding your selection.

1. Return to input screens. Change compound.
2. Return to input screens. Same compound.
3. Entered data are ok. Continue.

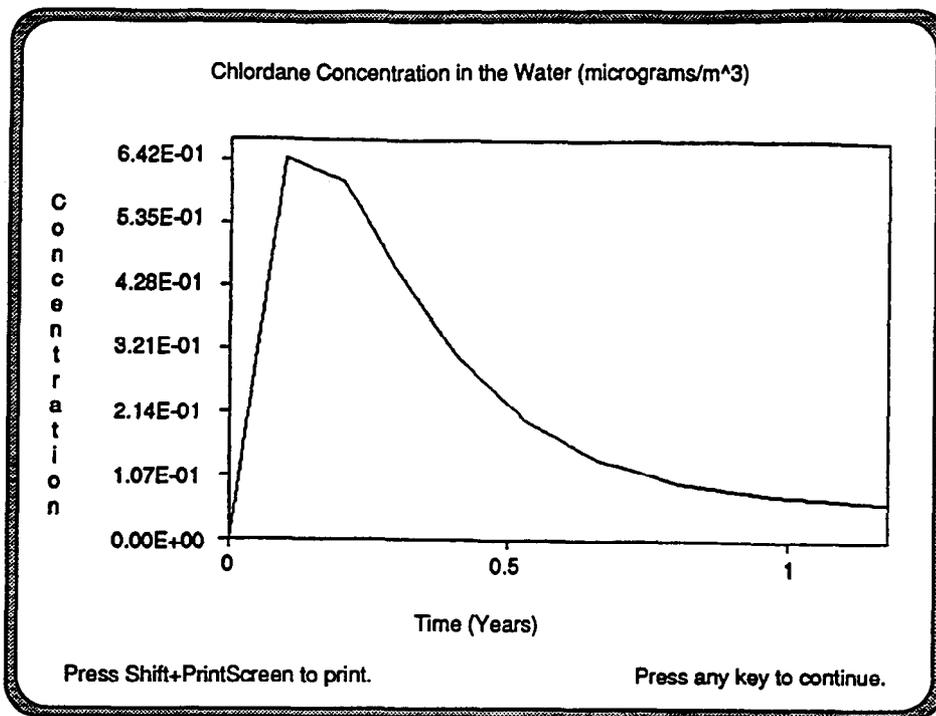
SCREEN 11



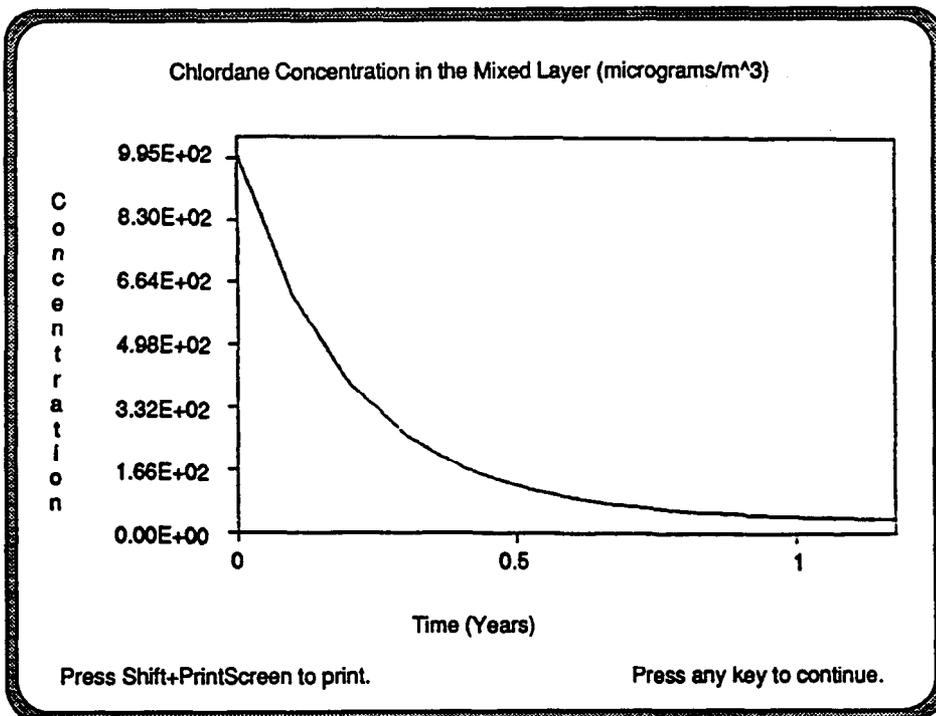
SCREEN 12

- Highlight your choice and press Enter or
press the number preceding your selection.
1. Plot Contaminant Concentration in Water.
 2. Plot Contaminant Concentration in Mixed Layer.
 3. Plot Flux of Contaminant from Sediments into Water.
 4. Plot Volatilization Rate from the Water.
 5. Print Table of Results to Printer.
 6. Return to Input Screens.
 7. Return to Beginning of Program.
 8. Save the Input Data for This Run.
 9. Exit Program.

SCREEN 13

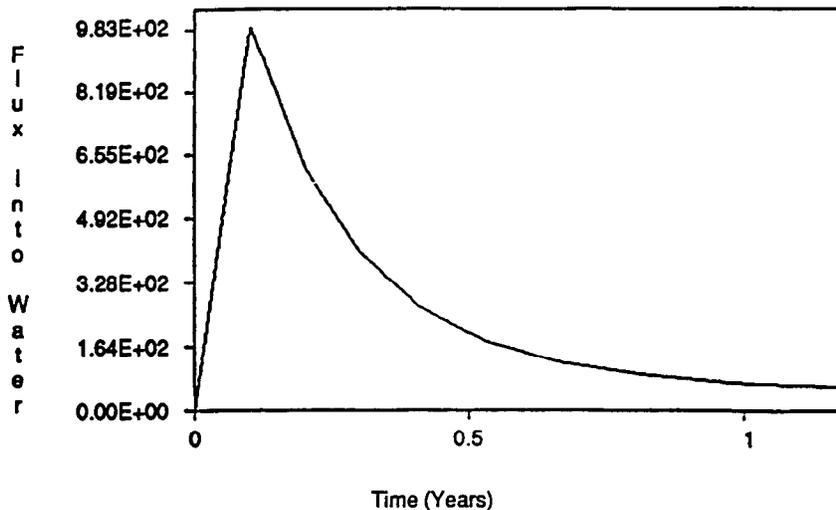


SCREEN 14



SCREEN 15

Flux of Chlordane into Water from Sediments (micrograms/(m²-yr))

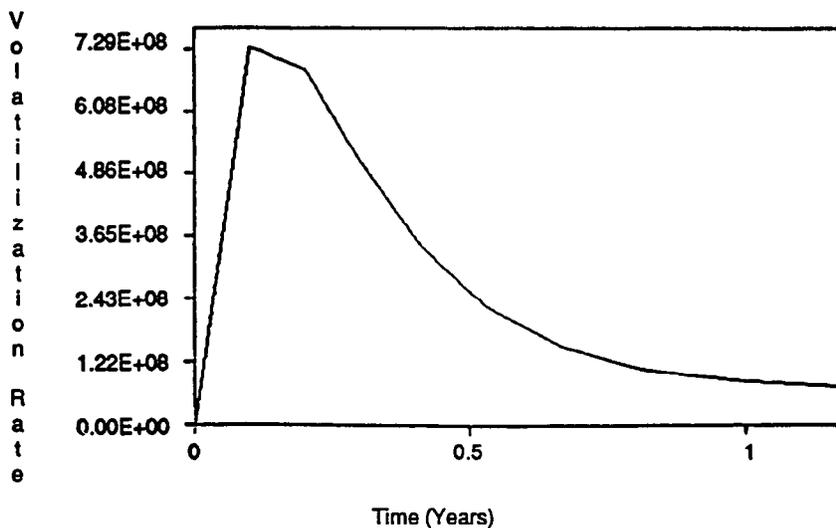


Press Shift+PrintScreen to print.

Press any key to continue.

SCREEN 16

Volatilization Rate Chlordane from the Water (micrograms/yr)



Press Shift+PrintScreen to print.

Press any key to continue.

SCREEN 17

REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

Public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden, to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302, and to the Office of Management and Budget, Paperwork Reduction Project (0704-0188), Washington, DC 20503.

1. AGENCY USE ONLY (Leave blank)	2. REPORT DATE November 1994	3. REPORT TYPE AND DATES COVERED Final report	
4. TITLE AND SUBTITLE RECOVERY, A Mathematical Model to Predict the Temporal Response of Surface Water to Contaminated Sediments		5. FUNDING NUMBERS	
6. AUTHOR(S) Jean M. Boyer, Steven C. Chapra Carlos E. Ruiz, Mark S. Dortch			
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) University of Colorado, Center for Advanced Decision Support for Water and Environmental Systems, Boulder CO 80309-0428; U.S. Army Engineer Waterways Experiment Station 3909 Halls Ferry Road, Vicksburg, MS 39180-6199		8. PERFORMING ORGANIZATION REPORT NUMBER Technical Report W-94-4	
9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES) U.S. Army Corps of Engineers, Washington, DC 20314-1000; U.S. Army Engineer Division, New England, Waltham, MA 02254-9149; U.S. Army Engineer District, New York, NY 10278-0090		10. SPONSORING / MONITORING AGENCY REPORT NUMBER	
11. SUPPLEMENTARY NOTES Available from National Technical Information Service, 5285 Port Royal Road, Springfield, VA 22161.			
12a. DISTRIBUTION / AVAILABILITY STATEMENT Approved for public release; distribution is unlimited.		12b. DISTRIBUTION CODE	
13. ABSTRACT (Maximum 200 words) RECOVERY is a PC-based screening-level model to assess the impact of contaminated bottom sediments on surface waters. The analysis is limited to organic contaminants with the assumption that the water column is well mixed. The contaminant is assumed to follow linear, reversible, equilibrium sorption and first-order decay kinetics. The physical representation of a system by RECOVERY consists of a well-mixed water column (i.e., zero-dimensional) underlain by a vertically stratified sediment column (i.e., one-dimensional). The sediment is well mixed horizontally, but segmented vertically into a well-mixed surface (active) layer and deep sediment. The deep sediment is segmented into contaminated and clean sediment regions. Pathways incorporated in the RECOVERY model, in addition to sorption and decay, are volatilization, burial, resuspension, settling, advection, and pore-water diffusion. RECOVERY is designed for interactive implementation via a personal computer. The program allows the user to rapidly generate and analyze recovery scenarios for contaminated sediments. The software includes graphical displays and is self-documented. A description of the model, a confirmation application, and a user's guide are included in this report.			
14. SUBJECT TERMS Contaminated sediments Organic contaminants Kinetics Partitioning Modeling Surface waters		15. NUMBER OF PAGES 61	
		16. PRICE CODE	
17. SECURITY CLASSIFICATION OF REPORT UNCLASSIFIED	18. SECURITY CLASSIFICATION OF THIS PAGE UNCLASSIFIED	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT